THE TORSIONAL SPECTRUM OF DOUBLY DEUTERATED METHANOL CHD_2OH

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Although the torsional spectrum of several isotopic species of methanol with a symmetrical CH_3 or CD_3 was analyzed some time ago, it is recently,[a] and only for the monodeuterated species CH_2DOH, that such an analysis was extended to the case of an asymmetrical methyl group.

In this talk, based on a Fourier transform high-resolution spectrum recorded in the 20 to 670 cm^{-1} region, the first analysis of the torsional spectrum of doubly deuterated methanol CHD_2OH will be presented. The Q branch of many torsional subbands could be observed and their assignment was initiated using a theoretical torsion-rotation spectrum computed with an approach accounting for the torsion-rotation Coriolis coupling and for the dependence of the generalized inertia tensor on the angle of internal rotation.[b] 46 torsional subbands were thus assigned. For 28 of them, their rotational structure could be assigned and fitted using an effective Hamiltonian expressed as a $J(J+1)$ expansion; and for 2 of them microwave transitions within the lower torsional level could also be included in the analysis.[c] In several cases these analysis revealed that the torsional levels are strongly perturbed.[d]

In the talk, the torsional parameters retrieved in the analysis of the torsional subband centers will be discussed. The results of the analysis of the rotational structure of the torsional subbands will be presented and we will also try to understand the nature of the perturbations. At last, preliminary results about the analysis of the microwave spectrum will be presented.

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[a] El Hilali, Coudert, Konov, and Klee, *J. Chem. Phys.* **135** (2011) 194309

[b] Lauvergnat, Coudert, Klee, and Smirnov, *J. Mol. Spectrosc.* **256** (2009) 204

[c] Quade, Liu, Mukhopadhyay, and Su, *J. Mol. Spectrosc.* **192** (1998) 378

[d] Pearson, Yu, and Drouin, *J. Mol. Spectrosc.* **280** (2012) 119